

(1R,2S,5R)-(-)-Menthol
2216-51-5 | DTXSID1022180

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 145 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.05e-01

Confidence level: 5.51e-01

Nearest Neighbors from the Training Set

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Decalin

Measured: 4680

Predicted: 4190

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Butanamide, N-phenyl-

Measured: 51.3

Predicted: 67.1

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1-Hydroxymethylnaphthalene

Measured: 148

Predicted: 406

Image not found

XMC

Measured: 51.3

Predicted: 79.8

Image not found

Isophorone

Measured: 25.1

Predicted: 103